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rac-12a,11b-Diphenyl-1,2,3,4,5,11-hexahydro-2,3,4a,5a,10a,11a-hexaazabenz[*f*]indeno[2,1,8-*ija*]naphth[2,3-*f*]azulene-1,4,10-trione chloroform solvate

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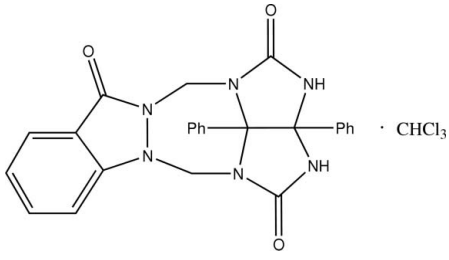
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.004 Å; disorder in solvent or counterion; R factor = 0.056; wR factor = 0.171; data-to-parameter ratio = 13.8.

The title compound, $C_{25}H_{20}N_6O_3\cdot CHCl_3$, a rigid glycoluril derivative, is an intermediate for the synthesis of molecular tweezers. The crystal structure is stabilized by intermolecular C—H···O and N—H···O hydrogen bonds. The chloroform solvent molecule is disordered over two positions; the site occupancy factors are *ca* 0.89 and 0.11.

Related literature

For related literature, see: Hof *et al.* (2002); Hu *et al.* (2007); Lagona *et al.* (2003); Li *et al.* (2006); Rebek (2005); Rowan *et al.* (1999); Wu *et al.* (2002); Yin *et al.* (2006).



Experimental

Crystal data

$C_{25}H_{20}N_6O_3.CHCl_3$
M_r = 571.84
Monoclinic, $P2_1/n$
a = 17.3315 (12) Å
b = 8.4507 (6) Å
c = 17.7874 (12) Å
β = 94.6520 (10)°
V = 2596.6 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.40 mm^{-1}
T = 292 (2) K
0.40 × 0.30 × 0.30 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
26236 measured reflections
5081 independent reflections
3995 reflections with $I > 2\sigma(I)$
R_{int} = 0.106

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.171
S = 1.12
5081 reflections
368 parameters
18 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5A···O1^{i}	0.857 (10)	2.42 (2)	3.004 (2)	126 (2)
N5—H5A···O2^{i}	0.857 (10)	2.11 (2)	2.782 (2)	135 (2)
N6—H6···O2^{i}	0.868 (10)	2.44 (2)	3.062 (2)	130 (2)
N6—H6···O1^{ii}	0.868 (10)	2.298 (17)	3.041 (2)	144 (2)
C8—H8A···O1	0.97	2.57	2.938 (3)	103
C14—H14···N3	0.93	2.51	2.832 (3)	101
C18—H18···N4	0.93	2.51	2.827 (3)	100
C21—H21···N5	0.93	2.48	2.821 (3)	102
C26—H26A···O1^{i}	0.98 (4)	2.43 (4)	3.364 (3)	158 (3)
C9—H9B···O3^{iii}	0.97	2.23	3.165 (2)	161

Symmetry codes: (i) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x, y+1, z$; (iii) $-x, -y+2, -z$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2109).

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supplementary materials

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rac-12a,11b-Diphenyl-1,2,3,4,5,11-hexahydro-2,3,4a,5a,10a,11a-hexaazabenz[*f*]indeno[2,1,8-*ija*]naphth[2,3-*f*]azulene-1,4,10-trione chloroform solvate

S.-L. Hu, J.-M. Zhang, G. Yan and S. Wang

Comment

The glycoluryl skeleton has served as an important building blocks for preparations of supramolecular systems including molecular clips (Rowan *et al.*, 1999; Yin *et al.*, 2006; Li *et al.*, 2006; Hu *et al.*, 2007), molecular capsules (Hof *et al.*, 2002; Rebek 2005) and the cucurbit[*n*]uryl family (Lagona *et al.*, 2003). Many methylene-bridged glycoluryl dimers have been synthesized by dimerization reaction of glycoluryl derivatives (Wu *et al.*, 2002). In this paper we report the crystal structure of the title compound (I).

The chirality of the molecule is induced by the inverted nitrogen atoms generating two chiral carbon atoms of the same absolute configuration (C12 and C19). The space group is centrosymmetric and the crystalline compound is a racemate. In the crystal structure of (I) (Fig. 1) the interplanar angle between the two five-membered rings C11/N4/C12/C19/N5 and C10/N3/C12/C19/N5 is 69.5 (1)° whereas the angle between the planes of the two benzene rings C13/C14/C15/C16/C17/C18 and C20/C21/C22/C23/C24/C25 is 66.4 (2) °. The aromatic ring (C1/C2/C3/C4/C5/C6) is coplanar with the five-membered (C1/C6/C7/N1/N2) ring. The molecules are connected by intermolecular C—H···O and N—H···O hydrogen bonds (Table 1and Fig. 2).

Experimental

The title compound was synthesized in analogy to the literature procedure of Lagona *et al.* (2003), Crystals appropriate for data collection were obtained by slow evaporation from a methanol-chloroform solution (1:20 V/V) of (I).

Refinement

The H atoms were constrained to an ideal geometry and constrained to ride on their parent atoms as follows: methylene H with d(C—H)=0.97 Å and U_{iso}(H) = 1.2U_{eq}(C); methine H with d(C—H)=0.98 Å and U_{iso}(H) = 1.2U_{eq}(C); aromatic H with d(C—H)=0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). The solvent molecule chloroform is disorder over two sites; the site-occupancy factors for the two orientations were refined by *DFIX*, giving 0.891 (4) and 0.109 (4) for the major and minor components, respectively.

Figures

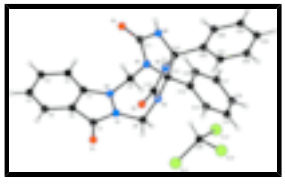

Fig. 1. View of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms atoms shown as circles of arbitrary radii. Higher populated orientation of disordered solvate molecule is shown.

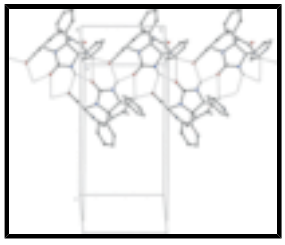

Fig. 2. The molecular packing of (I) viewed along the *b* axis.

rac-12*a*,11*b*-Diphenyl-1,2,3,4,5,11-hexahydro-2,3,4a,5a,10*a*,11*a*-hexaazabenz[*f*]\ indeno[2,1,8-ija]naphth[2,3-*f*]azulene-1,4,10-trione chloroform solvate

Crystal data

$C_{25}H_{20}N_6O_3.CHCl_3$	F_{000} = 1176
M_r = 571.84	D_x = 1.463 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 9009 reflections
a = 17.3315 (12) Å	θ = 2.3–26.2º
b = 8.4507 (6) Å	μ = 0.40 mm^{-1}
c = 17.7874 (12) Å	T = 292 (2) K
β = 94.6520 (10)º	Block, colourless
V = 2596.6 (3) Å^3	0.40 × 0.30 × 0.30 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	3995 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.106
Monochromator: graphite	θ_{max} = 26.0º
T = 292(2) K	θ_{min} = 2.3º
φ and ω scans	h = −21→21
Absorption correction: none	k = −10→10
26236 measured reflections	l = −21→21
5081 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.056	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.171	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 0.1644P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.12	$(\Delta/\sigma)_{max} < 0.001$
5081 reflections	$\Delta\rho_{max}$ = 0.55 e Å^{-3}

368 parameters
18 restraints
Primary atom site location: structure-invariant direct methods

$\Delta\rho_{min} = -0.45$ e Å^{-3}
Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	−0.01228 (12)	0.6113 (2)	0.09136 (11)	0.0406 (5)	
C2	−0.08340 (13)	0.6849 (3)	0.07437 (13)	0.0512 (6)	
H2	−0.0897	0.7649	0.0385	0.061*	
C3	−0.14406 (14)	0.6327 (3)	0.11352 (14)	0.0579 (6)	
H3	−0.1925	0.6790	0.1037	0.070*	
C4	−0.13512 (15)	0.5126 (3)	0.16741 (14)	0.0614 (7)	
H4	−0.1777	0.4796	0.1919	0.074*	
C5	−0.06507 (15)	0.4427 (3)	0.18466 (13)	0.0548 (6)	
H5	−0.0592	0.3637	0.2211	0.066*	
C6	−0.00201 (13)	0.4933 (2)	0.14600 (11)	0.0416 (5)	
C7	0.07793 (12)	0.4425 (2)	0.15020 (11)	0.0401 (5)	
C8	0.19109 (11)	0.5352 (2)	0.08132 (11)	0.0364 (4)	
H8A	0.2180	0.4513	0.1099	0.044*	
H8B	0.1949	0.5134	0.0282	0.044*	
C9	0.07849 (11)	0.7535 (2)	0.00801 (11)	0.0366 (4)	
H9A	0.0997	0.7030	−0.0348	0.044*	
H9B	0.0327	0.8116	−0.0108	0.044*	
C10	0.24996 (12)	0.7221 (2)	0.17428 (11)	0.0383 (4)	
C11	0.11468 (11)	0.9955 (2)	0.08124 (10)	0.0358 (4)	
C12	0.21600 (10)	0.8227 (2)	0.05273 (10)	0.0313 (4)	
C13	0.25256 (11)	0.8065 (2)	−0.02170 (10)	0.0365 (4)	
C14	0.31630 (13)	0.7111 (3)	−0.02762 (13)	0.0485 (5)	
H14	0.3367	0.6539	0.0140	0.058*	
C15	0.35027 (16)	0.7001 (3)	−0.09556 (16)	0.0656 (7)	
H15	0.3932	0.6354	−0.0990	0.079*	
C16	0.32150 (18)	0.7826 (4)	−0.15692 (15)	0.0730 (8)	
H16	0.3443	0.7735	−0.2023	0.088*	
C17	0.25842 (18)	0.8798 (4)	−0.15183 (15)	0.0716 (8)	
H17	0.2390	0.9378	−0.1936	0.086*	

C18	0.22375 (14)	0.8913 (3)	−0.08427 (12)	0.0513 (6)	
H18	0.1809	0.9565	−0.0811	0.062*	
C19	0.24895 (11)	0.9617 (2)	0.10817 (10)	0.0337 (4)	
C20	0.31752 (12)	1.0523 (2)	0.08231 (12)	0.0405 (5)	
C21	0.39225 (14)	1.0119 (3)	0.10742 (17)	0.0604 (6)	
H21	0.4010	0.9328	0.1435	0.073*	
C22	0.45422 (17)	1.0884 (4)	0.0792 (2)	0.0852 (10)	
H22	0.5045	1.0594	0.0958	0.102*	
C23	0.4419 (2)	1.2067 (5)	0.0271 (2)	0.0919 (11)	
H23	0.4838	1.2583	0.0085	0.110*	
C24	0.3686 (2)	1.2488 (4)	0.00243 (19)	0.0841 (10)	
H24	0.3605	1.3292	−0.0330	0.101*	
C25	0.30584 (16)	1.1725 (3)	0.02971 (15)	0.0579 (6)	
H25	0.2558	1.2022	0.0127	0.069*	
C26	0.46631 (16)	0.5204 (3)	0.23715 (15)	0.0657 (7)	
H26A	0.443 (2)	0.596 (4)	0.270 (2)	0.079*	0.89
H26B	0.4541 (8)	0.5929 (15)	0.2749 (7)	0.079*	0.11
Cl1	0.41377 (9)	0.34312 (14)	0.23910 (8)	0.1022 (6)	0.891 (4)
Cl2	0.56162 (7)	0.4907 (3)	0.27090 (7)	0.1030 (6)	0.891 (4)
Cl3	0.46003 (13)	0.59902 (19)	0.14665 (6)	0.1049 (6)	0.891 (4)
Cl1'	0.3909 (5)	0.4067 (16)	0.2006 (8)	0.128 (5)*	0.109 (4)
Cl2'	0.5452 (5)	0.4011 (15)	0.2668 (6)	0.099 (4)*	0.109 (4)
Cl3'	0.5003 (8)	0.6358 (12)	0.1606 (6)	0.106 (4)*	0.109 (4)
N1	0.11038 (9)	0.53202 (19)	0.09645 (9)	0.0394 (4)	
N2	0.05607 (9)	0.6324 (2)	0.05924 (11)	0.0449 (4)	
N3	0.22939 (9)	0.68300 (17)	0.09983 (8)	0.0336 (4)	
N4	0.13463 (9)	0.86380 (18)	0.04135 (9)	0.0346 (4)	
N5	0.26771 (11)	0.8756 (2)	0.17713 (9)	0.0426 (4)	
N6	0.18148 (10)	1.0629 (2)	0.11157 (10)	0.0401 (4)	
O1	0.11387 (9)	0.34349 (17)	0.19079 (9)	0.0515 (4)	
O2	0.25289 (11)	0.62845 (19)	0.22639 (8)	0.0567 (5)	
O3	0.04941 (8)	1.04336 (18)	0.08530 (8)	0.0476 (4)	
H6	0.1812 (15)	1.133 (2)	0.1474 (11)	0.057*	
H5A	0.2804 (14)	0.920 (3)	0.2196 (9)	0.057*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0391 (11)	0.0430 (11)	0.0388 (11)	−0.0064 (8)	−0.0024 (8)	−0.0056 (8)
C2	0.0422 (12)	0.0570 (14)	0.0530 (13)	−0.0005 (10)	−0.0038 (10)	0.0019 (10)
C3	0.0409 (12)	0.0740 (16)	0.0588 (15)	0.0014 (11)	0.0031 (11)	−0.0066 (12)
C4	0.0514 (14)	0.0790 (18)	0.0560 (15)	−0.0111 (13)	0.0173 (11)	−0.0100 (13)
C5	0.0602 (15)	0.0600 (14)	0.0449 (13)	−0.0103 (11)	0.0082 (10)	0.0001 (10)
C6	0.0469 (12)	0.0424 (11)	0.0348 (10)	−0.0067 (9)	−0.0001 (8)	−0.0049 (8)
C7	0.0466 (11)	0.0359 (10)	0.0364 (10)	−0.0057 (8)	−0.0051 (8)	−0.0004 (8)
C8	0.0376 (10)	0.0318 (10)	0.0388 (10)	0.0017 (8)	−0.0033 (8)	−0.0017 (8)
C9	0.0349 (10)	0.0434 (11)	0.0305 (9)	0.0003 (8)	−0.0046 (7)	0.0028 (8)
C10	0.0414 (11)	0.0392 (10)	0.0331 (10)	−0.0020 (8)	−0.0045 (8)	0.0019 (8)

C11	0.0399 (11)	0.0390 (10)	0.0285 (9)	0.0033 (8)	0.0025 (7)	0.0036 (7)
C12	0.0323 (9)	0.0320 (9)	0.0290 (9)	0.0006 (7)	−0.0016 (7)	−0.0005 (7)
C13	0.0375 (10)	0.0398 (10)	0.0323 (10)	−0.0046 (8)	0.0024 (8)	−0.0029 (8)
C14	0.0437 (12)	0.0572 (13)	0.0449 (12)	0.0042 (10)	0.0066 (9)	−0.0007 (10)
C15	0.0526 (15)	0.0804 (18)	0.0671 (17)	0.0074 (13)	0.0247 (12)	−0.0071 (14)
C16	0.0769 (19)	0.098 (2)	0.0480 (15)	0.0016 (17)	0.0300 (13)	0.0021 (14)
C17	0.0815 (19)	0.095 (2)	0.0406 (13)	0.0067 (16)	0.0161 (13)	0.0168 (13)
C18	0.0557 (13)	0.0604 (14)	0.0383 (12)	0.0059 (11)	0.0074 (10)	0.0079 (10)
C19	0.0362 (10)	0.0333 (9)	0.0307 (9)	0.0010 (7)	−0.0020 (7)	−0.0008 (7)
C20	0.0407 (11)	0.0360 (10)	0.0449 (11)	−0.0052 (8)	0.0047 (9)	−0.0064 (8)
C21	0.0445 (13)	0.0547 (14)	0.0811 (18)	−0.0027 (10)	−0.0009 (12)	−0.0069 (12)
C22	0.0457 (15)	0.092 (2)	0.120 (3)	−0.0150 (15)	0.0184 (16)	−0.028 (2)
C23	0.077 (2)	0.098 (2)	0.106 (3)	−0.040 (2)	0.039 (2)	−0.019 (2)
C24	0.108 (3)	0.0687 (19)	0.079 (2)	−0.0324 (18)	0.0289 (18)	0.0080 (15)
C25	0.0628 (15)	0.0493 (13)	0.0619 (15)	−0.0099 (11)	0.0066 (12)	0.0081 (11)
C26	0.0740 (17)	0.0701 (17)	0.0544 (15)	0.0191 (14)	0.0131 (12)	−0.0052 (13)
Cl1	0.1324 (10)	0.0798 (7)	0.0974 (9)	−0.0179 (6)	0.0280 (7)	−0.0191 (6)
Cl2	0.0727 (7)	0.1422 (15)	0.0931 (8)	0.0284 (7)	0.0004 (5)	−0.0072 (7)
Cl3	0.1443 (14)	0.1069 (9)	0.0636 (6)	0.0391 (9)	0.0090 (7)	0.0229 (5)
N1	0.0385 (9)	0.0366 (9)	0.0418 (9)	−0.0007 (7)	−0.0050 (7)	0.0047 (7)
N2	0.0320 (9)	0.0491 (10)	0.0530 (11)	−0.0022 (7)	−0.0008 (7)	0.0133 (8)
N3	0.0391 (9)	0.0307 (8)	0.0300 (8)	0.0003 (6)	−0.0040 (6)	0.0006 (6)
N4	0.0322 (8)	0.0381 (8)	0.0328 (8)	0.0025 (6)	−0.0025 (6)	−0.0021 (6)
N5	0.0582 (11)	0.0375 (9)	0.0298 (9)	−0.0048 (8)	−0.0097 (8)	−0.0003 (7)
N6	0.0420 (9)	0.0373 (9)	0.0410 (9)	0.0036 (7)	0.0022 (7)	−0.0093 (7)
O1	0.0560 (10)	0.0462 (8)	0.0508 (9)	−0.0017 (7)	−0.0054 (7)	0.0123 (7)
O2	0.0823 (12)	0.0475 (9)	0.0372 (8)	−0.0149 (8)	−0.0140 (8)	0.0126 (7)
O3	0.0375 (8)	0.0588 (9)	0.0463 (8)	0.0139 (7)	0.0022 (6)	−0.0015 (7)

Geometric parameters (Å, °)

C1—N2	1.368 (3)	C14—C15	1.390 (3)
C1—C2	1.392 (3)	C14—H14	0.9300
C1—C6	1.394 (3)	C15—C16	1.355 (4)
C2—C3	1.380 (3)	C15—H15	0.9300
C2—H2	0.9300	C16—C17	1.376 (4)
C3—C4	1.396 (4)	C16—H16	0.9300
C3—H3	0.9300	C17—C18	1.390 (3)
C4—C5	1.362 (4)	C17—H17	0.9300
C4—H4	0.9300	C18—H18	0.9300
C5—C6	1.404 (3)	C19—N5	1.440 (2)
C5—H5	0.9300	C19—N6	1.454 (2)
C6—C7	1.446 (3)	C19—C20	1.516 (3)
C7—O1	1.240 (2)	C20—C21	1.378 (3)
C7—N1	1.375 (3)	C20—C25	1.385 (3)
C8—N3	1.440 (2)	C21—C22	1.382 (4)
C8—N1	1.446 (3)	C21—H21	0.9300
C8—H8A	0.9700	C22—C23	1.369 (5)
C8—H8B	0.9700	C22—H22	0.9300

C9—N4	1.440 (2)	C23—C24	1.357 (5)
C9—N2	1.444 (2)	C23—H23	0.9300
C9—H9A	0.9700	C24—C25	1.386 (4)
C9—H9B	0.9700	C24—H24	0.9300
C10—O2	1.217 (2)	C25—H25	0.9300
C10—N5	1.333 (3)	C26—Cl1'	1.707 (7)
C10—N3	1.383 (2)	C26—Cl2	1.730 (3)
C11—O3	1.209 (2)	C26—Cl3	1.737 (3)
C11—N6	1.362 (3)	C26—Cl2'	1.746 (6)
C11—N4	1.379 (2)	C26—Cl1	1.755 (3)
C12—N4	1.450 (2)	C26—Cl3'	1.811 (7)
C12—N3	1.456 (2)	C26—H26A	0.98 (4)
C12—C13	1.520 (3)	C26—H26B	0.945 (8)
C12—C19	1.608 (2)	N1—N2	1.394 (2)
C13—C14	1.378 (3)	N5—H5A	0.857 (10)
C13—C18	1.382 (3)	N6—H6	0.868 (10)
N2—C1—C2	129.3 (2)	N6—C19—C12	102.02 (14)
N2—C1—C6	108.56 (18)	C20—C19—C12	115.52 (15)
C2—C1—C6	122.1 (2)	C21—C20—C25	118.9 (2)
C3—C2—C1	116.5 (2)	C21—C20—C19	121.0 (2)
C3—C2—H2	121.8	C25—C20—C19	120.0 (2)
C1—C2—H2	121.8	C20—C21—C22	120.2 (3)
C2—C3—C4	122.2 (2)	C20—C21—H21	119.9
C2—C3—H3	118.9	C22—C21—H21	119.9
C4—C3—H3	118.9	C23—C22—C21	120.3 (3)
C5—C4—C3	121.1 (2)	C23—C22—H22	119.8
C5—C4—H4	119.4	C21—C22—H22	119.8
C3—C4—H4	119.4	C24—C23—C22	120.0 (3)
C4—C5—C6	118.2 (2)	C24—C23—H23	120.0
C4—C5—H5	120.9	C22—C23—H23	120.0
C6—C5—H5	120.9	C23—C24—C25	120.4 (3)
C1—C6—C5	119.9 (2)	C23—C24—H24	119.8
C1—C6—C7	108.41 (18)	C25—C24—H24	119.8
C5—C6—C7	131.7 (2)	C20—C25—C24	120.1 (3)
O1—C7—N1	124.20 (19)	C20—C25—H25	120.0
O1—C7—C6	131.6 (2)	C24—C25—H25	120.0
N1—C7—C6	104.19 (16)	Cl1'—C26—Cl2	136.9 (5)
N3—C8—N1	114.13 (16)	Cl1'—C26—Cl3	82.8 (5)
N3—C8—H8A	108.7	Cl2—C26—Cl3	111.31 (17)
N1—C8—H8A	108.7	Cl1'—C26—Cl2'	110.3 (5)
N3—C8—H8B	108.7	Cl2—C26—Cl2'	26.9 (4)
N1—C8—H8B	108.7	Cl3—C26—Cl2'	119.3 (4)
H8A—C8—H8B	107.6	Cl1'—C26—Cl1	31.2 (5)
N4—C9—N2	113.96 (15)	Cl2—C26—Cl1	110.59 (16)
N4—C9—H9A	108.8	Cl3—C26—Cl1	110.56 (17)
N2—C9—H9A	108.8	Cl2'—C26—Cl1	84.0 (4)
N4—C9—H9B	108.8	Cl1'—C26—Cl3'	107.6 (5)
N2—C9—H9B	108.8	Cl2—C26—Cl3'	88.8 (4)
H9A—C9—H9B	107.7	Cl3—C26—Cl3'	25.5 (4)

O2—C10—N5	127.50 (18)	Cl2'—C26—Cl3'	104.1 (4)
O2—C10—N3	124.42 (19)	Cl1—C26—Cl3'	132.5 (5)
N5—C10—N3	108.05 (16)	Cl1'—C26—H26A	105 (2)
O3—C11—N6	127.32 (18)	Cl2—C26—H26A	108 (2)
O3—C11—N4	125.12 (18)	Cl3—C26—H26A	108 (2)
N6—C11—N4	107.51 (17)	Cl2'—C26—H26A	123 (2)
N4—C12—N3	112.47 (15)	Cl1—C26—H26A	108 (2)
N4—C12—C13	111.68 (14)	Cl3'—C26—H26A	106 (2)
N3—C12—C13	111.72 (15)	Cl1'—C26—H26B	115.3 (8)
N4—C12—C19	101.76 (13)	Cl2—C26—H26B	96.3 (9)
N3—C12—C19	101.96 (13)	Cl3—C26—H26B	114.2 (9)
C13—C12—C19	116.60 (15)	Cl2'—C26—H26B	112.0 (8)
C14—C13—C18	118.75 (19)	Cl1—C26—H26B	113.1 (9)
C14—C13—C12	120.85 (18)	Cl3'—C26—H26B	106.9 (8)
C18—C13—C12	120.38 (18)	H26A—C26—H26B	12 (2)
C13—C14—C15	120.3 (2)	C7—N1—N2	111.51 (16)
C13—C14—H14	119.9	C7—N1—C8	126.60 (16)
C15—C14—H14	119.9	N2—N1—C8	121.76 (16)
C16—C15—C14	120.8 (2)	C1—N2—N1	107.27 (16)
C16—C15—H15	119.6	C1—N2—C9	129.95 (17)
C14—C15—H15	119.6	N1—N2—C9	121.67 (15)
C15—C16—C17	119.8 (2)	C10—N3—C8	120.30 (16)
C15—C16—H16	120.1	C10—N3—C12	111.95 (15)
C17—C16—H16	120.1	C8—N3—C12	121.53 (14)
C16—C17—C18	120.0 (2)	C11—N4—C9	123.04 (16)
C16—C17—H17	120.0	C11—N4—C12	113.75 (15)
C18—C17—H17	120.0	C9—N4—C12	121.30 (15)
C13—C18—C17	120.4 (2)	C10—N5—C19	115.06 (16)
C13—C18—H18	119.8	C10—N5—H5A	120.2 (18)
C17—C18—H18	119.8	C19—N5—H5A	123.6 (18)
N5—C19—N6	112.86 (16)	C11—N6—C19	113.47 (16)
N5—C19—C20	112.66 (16)	C11—N6—H6	121.3 (17)
N6—C19—C20	111.60 (16)	C19—N6—H6	118.8 (18)
N5—C19—C12	101.41 (14)		
N2—C1—C2—C3	176.2 (2)	C23—C24—C25—C20	−0.2 (5)
C6—C1—C2—C3	−1.2 (3)	O1—C7—N1—N2	179.60 (18)
C1—C2—C3—C4	0.0 (4)	C6—C7—N1—N2	−0.6 (2)
C2—C3—C4—C5	1.1 (4)	O1—C7—N1—C8	−4.5 (3)
C3—C4—C5—C6	−0.9 (4)	C6—C7—N1—C8	175.28 (17)
N2—C1—C6—C5	−176.52 (19)	N3—C8—N1—C7	−112.6 (2)
C2—C1—C6—C5	1.4 (3)	N3—C8—N1—N2	62.9 (2)
N2—C1—C6—C7	2.4 (2)	C2—C1—N2—N1	179.6 (2)
C2—C1—C6—C7	−179.69 (19)	C6—C1—N2—N1	−2.7 (2)
C4—C5—C6—C1	−0.3 (3)	C2—C1—N2—C9	11.7 (4)
C4—C5—C6—C7	−178.9 (2)	C6—C1—N2—C9	−170.53 (19)
C1—C6—C7—O1	178.7 (2)	C7—N1—N2—C1	2.1 (2)
C5—C6—C7—O1	−2.6 (4)	C8—N1—N2—C1	−174.03 (17)
C1—C6—C7—N1	−1.1 (2)	C7—N1—N2—C9	171.13 (17)
C5—C6—C7—N1	177.6 (2)	C8—N1—N2—C9	−5.0 (3)

N4—C12—C13—C14	−153.83 (18)	N4—C9—N2—C1	109.2 (2)
N3—C12—C13—C14	−26.9 (2)	N4—C9—N2—N1	−57.1 (2)
C19—C12—C13—C14	89.8 (2)	O2—C10—N3—C8	15.8 (3)
N4—C12—C13—C18	28.2 (3)	N5—C10—N3—C8	−166.13 (17)
N3—C12—C13—C18	155.12 (19)	O2—C10—N3—C12	168.5 (2)
C19—C12—C13—C18	−88.2 (2)	N5—C10—N3—C12	−13.4 (2)
C18—C13—C14—C15	−0.5 (3)	N1—C8—N3—C10	75.2 (2)
C12—C13—C14—C15	−178.5 (2)	N1—C8—N3—C12	−74.9 (2)
C13—C14—C15—C16	0.0 (4)	N4—C12—N3—C10	−97.09 (18)
C14—C15—C16—C17	0.7 (5)	C13—C12—N3—C10	136.40 (17)
C15—C16—C17—C18	−1.0 (5)	C19—C12—N3—C10	11.15 (19)
C14—C13—C18—C17	0.2 (4)	N4—C12—N3—C8	55.2 (2)
C12—C13—C18—C17	178.3 (2)	C13—C12—N3—C8	−71.3 (2)
C16—C17—C18—C13	0.5 (4)	C19—C12—N3—C8	163.46 (16)
N4—C12—C19—N5	111.33 (15)	O3—C11—N4—C9	−9.1 (3)
N3—C12—C19—N5	−4.98 (18)	N6—C11—N4—C9	173.40 (16)
C13—C12—C19—N5	−126.92 (17)	O3—C11—N4—C12	−173.50 (18)
N4—C12—C19—N6	−5.30 (17)	N6—C11—N4—C12	9.0 (2)
N3—C12—C19—N6	−121.60 (15)	N2—C9—N4—C11	−85.1 (2)
C13—C12—C19—N6	116.45 (17)	N2—C9—N4—C12	78.2 (2)
N4—C12—C19—C20	−126.54 (16)	N3—C12—N4—C11	106.46 (17)
N3—C12—C19—C20	117.15 (17)	C13—C12—N4—C11	−127.01 (16)
C13—C12—C19—C20	−4.8 (2)	C19—C12—N4—C11	−1.91 (19)
N5—C19—C20—C21	20.5 (3)	N3—C12—N4—C9	−58.2 (2)
N6—C19—C20—C21	148.6 (2)	C13—C12—N4—C9	68.3 (2)
C12—C19—C20—C21	−95.4 (2)	C19—C12—N4—C9	−166.61 (15)
N5—C19—C20—C25	−162.89 (19)	O2—C10—N5—C19	−172.2 (2)
N6—C19—C20—C25	−34.7 (3)	N3—C10—N5—C19	9.9 (2)
C12—C19—C20—C25	81.2 (2)	N6—C19—N5—C10	105.7 (2)
C25—C20—C21—C22	−1.2 (4)	C20—C19—N5—C10	−126.81 (19)
C19—C20—C21—C22	175.4 (2)	C12—C19—N5—C10	−2.7 (2)
C20—C21—C22—C23	1.0 (5)	O3—C11—N6—C19	169.48 (19)
C21—C22—C23—C24	−0.4 (5)	N4—C11—N6—C19	−13.1 (2)
C22—C23—C24—C25	0.0 (5)	N5—C19—N6—C11	−96.61 (19)
C21—C20—C25—C24	0.8 (4)	C20—C19—N6—C11	135.33 (17)
C19—C20—C25—C24	−175.9 (2)	C12—C19—N6—C11	11.4 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5A···O1^{i}	0.857 (10)	2.42 (2)	3.004 (2)	126 (2)
N5—H5A···O2^{i}	0.857 (10)	2.11 (2)	2.782 (2)	135 (2)
N6—H6···O2^{i}	0.868 (10)	2.44 (2)	3.062 (2)	130 (2)
N6—H6···O1^{ii}	0.868 (10)	2.298 (17)	3.041 (2)	144 (2)
C8—H8A···O1	0.97	2.57	2.938 (3)	103
C14—H14···N3	0.93	2.51	2.832 (3)	101
C18—H18···N4	0.93	2.51	2.827 (3)	100
C21—H21···N5	0.93	2.48	2.821 (3)	102

C26—H26A···O1^{i}	0.98 (4)	2.43 (4)	3.364 (3)	158 (3)
C9—H9B···O3^{iii}	0.97	2.23	3.165 (2)	161

Symmetry codes: (i) −*x*+1/2, *y*+1/2, −*z*+1/2; (ii) *x*, *y*+1, *z*; (iii) −*x*, −*y*+2, −*z*.

Fig. 1

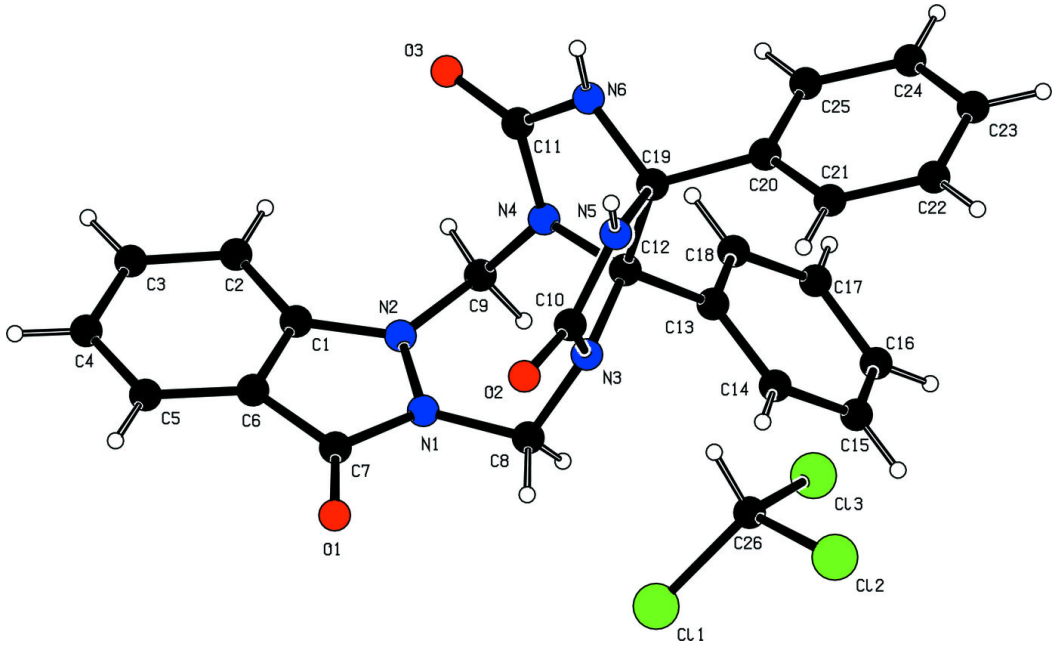
O3
N6
C11
C19
C25
C24
C23
C20
C21
C22
N4
N5
C12
C18
C17
C3
C2
N2
C9
C10
C13
C16
C1
C4
O2
N3
C14
C5
C6
N1
C8
C15
C7
Cl3
C26
O1
Cl2
Cl1

Fig. 2